CMA-ES and Advanced Adaptation Mechanisms

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We are happy to answer questions at any time.

1. Problem Statement
2. Evolution Strategy (ES)
3. Step-Size Adaptation
   - Why Step-Size Control
   - Path Length Control (CSA)
   - Limitations of CSA and its Alternatives
4. Covariance Matrix Adaptation (CMA)
   - Rank-One Update and Cumulation
   - Rank-μ Update
   - Active Covariance Update
5. Design Principle
   - Theoretical Foundations
   - Variants for Large Scale Problems
6. Summary and Final Remarks

Problem Statement

Continuous Domain Search/Optimization

- Task: minimize an objective function (*fitness* function, *loss* function) in continuous domain

$$f : \mathcal{X} \subseteq \mathbb{R}^n \to \mathbb{R}, \qquad \boldsymbol{x} \mapsto f(\boldsymbol{x})$$

- Black Box scenario (direct search scenario)

  - gradients are not available or not useful
  - problem domain specific knowledge is used only within the black box, e.g. within an appropriate encoding
- Search costs: number of function evaluations

Problem Statement

Continuous Domain Search/Optimization

- Goal
  - fast convergence to the global optimum
  - solution $\boldsymbol{x}$ with small function value $f(\boldsymbol{x})$ with least search cost

    . . . or to a robust solution $\boldsymbol{x}$

    there are two conflicting objectives
- Typical Examples
  - shape optimization (e.g. using CFD) — curve fitting, airfoils
  - model calibration — biological, physical
  - parameter calibration — controller, plants, images
- Problems
  - exhaustive search is infeasible
  - naive random search takes too long
  - deterministic search is not successful / takes too long

Approach: stochastic search, Evolutionary Algorithms

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Objective Function Properties

We assume $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ to be *non-linear, non-separable* and to have at least moderate dimensionality, say $n \not\ll 10$.

Additionally, f can be

- non-convex
- multimodal

  there are possibly many local optima
- non-smooth

  derivatives do not exist
- discontinuous, plateaus
- ill-conditioned
- noisy
- . . .

Goal : cope with any of these function properties

they are related to real-world problems

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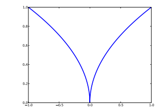
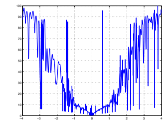
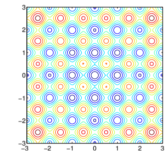
What Makes a Function Difficult to Solve?

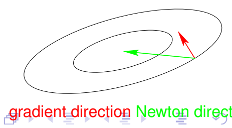
Why stochastic search?

- non-linear, non-quadratic, non-convex
  on linear and quadratic functions much better search policies are available
- ruggedness
  non-smooth, discontinuous, multimodal, and/or noisy function
- dimensionality (size of search space)
  (considerably) larger than three
- non-separability
  dependencies between the objective variables
- ill-conditioning









What Makes a Function Difficult to Solve?

... and what can be done

The Problem	Possible Approaches
Dimensionality	exploiting the problem structure separability, locality/neighborhood, encoding
Ill-conditioning	second order approach changes the neighborhood metric
Ruggedness	non-local policy, large sampling width (step-size) as large as possible while preserving a reasonable convergence speed
	population-based method, stochastic, non-elitistic
	recombination operator serves as repair mechanism
	restarts

... metaphors

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Stochastic Search

A black box search template to minimize $f : \mathbb{R}^n \to \mathbb{R}$

Initialize distribution parameters θ, set population size $\lambda \in \mathbb{N}$
While not terminate

1. Sample distribution $P(\boldsymbol{x}|\theta) \to \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda \in \mathbb{R}^n$
2. Evaluate $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda$ on f
3. Update parameters $\theta \leftarrow F_\theta(\theta, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_\lambda))$

Everything depends on the definition of P and F_θ

deterministic algorithms are covered as well

In many Evolutionary Algorithms the distribution P is implicitly defined via operators on a population, in particular, selection, recombination and mutation

Natural template for (incremental) *Estimation of Distribution Algorithms*

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The CMA-ES

Input: $\boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, λ
Initialize: $\mathbf{C} = \mathbf{I}$, and $\boldsymbol{p}_c = \mathbf{0}$, $\boldsymbol{p}_\sigma = \mathbf{0}$,
Set: $c_c \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \le 1$, $d_\sigma \approx 1 + \sqrt{\frac{\mu_w}{n}}$,
and $w_{i=1\ldots\lambda}$ such that $\mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i{}^2} \approx 0.3\,\lambda$

While not terminate

$$\boldsymbol{x}_i = \boldsymbol{m} + \sigma\, \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \quad \text{for } i = 1, \ldots, \lambda \qquad \text{sampling}$$

$$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i\, \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma\, \boldsymbol{y}_w \quad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i\, \boldsymbol{y}_{i:\lambda} \qquad \text{update mean}$$

$$\boldsymbol{p}_c \leftarrow (1 - c_c)\, \boldsymbol{p}_c + \mathbb{1}_{\{\|\boldsymbol{p}_\sigma\| < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, \boldsymbol{y}_w \qquad \text{cumulation for } \mathbf{C}$$

$$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\, \boldsymbol{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} \boldsymbol{y}_w \qquad \text{cumulation for } \sigma$$

$$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_1\, \boldsymbol{p}_c \boldsymbol{p}_c{}^{\mathrm{T}} + c_\mu \sum_{i=1}^{\mu} w_i\, \boldsymbol{y}_{i:\lambda} \boldsymbol{y}_{i:\lambda}^{\mathrm{T}} \qquad \text{update } \mathbf{C}$$

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right) \qquad \text{update of } \sigma$$

Not covered on this slide: termination, restarts, useful output, boundaries and encoding

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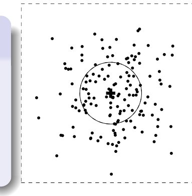
Evolution Strategies

New search points are sampled normally distributed

$$x_i \sim m + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of m, where $x_i, m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



where

- the mean vector $m \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

here, all new points are sampled with the same parameters

The question remains how to update m, $\mathbf{C}$, and σ.

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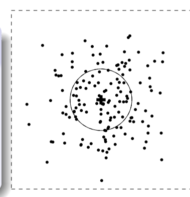

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Evolution Strategies

Terminology

Let μ: # of parents, λ: # of offspring

Plus (elitist) and comma (non-elitist) selection

$(\mu + \lambda)$-ES: selection in $\{$parents$\} \cup \{$offspring$\}$

(μ, λ)-ES: selection in $\{$offspring$\}$

$(1+1)$-ES

Sample one offspring from parent m

$$x = m + \sigma \mathcal{N}(\mathbf{0}, \mathbf{C})$$

If x better than m select

$$m \leftarrow x$$

why?

The $(\mu/\mu, \lambda)$-ES

Non-elitist selection and intermediate (weighted) recombination

Given the i-th solution point $\boldsymbol{x}_i = \boldsymbol{m} + \sigma \underbrace{\mathcal{N}_i(\mathbf{0}, \mathbf{C})}_{=:\boldsymbol{y}_i} = \boldsymbol{m} + \sigma\, \boldsymbol{y}_i$

Let $\boldsymbol{x}_{i:\lambda}$ the i-th ranked solution point, such that $f(\boldsymbol{x}_{1:\lambda}) \leq \cdots \leq f(\boldsymbol{x}_{\lambda:\lambda})$.
The new mean reads

$$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i\, \boldsymbol{x}_{i:\lambda}$$

where

$$w_1 \geq \cdots \geq w_\mu > 0, \quad \sum_{i=1}^{\mu} w_i = 1, \quad \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} =: \mu_w \approx \frac{\lambda}{4}$$

The best μ points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

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Recalling

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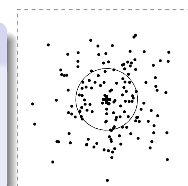

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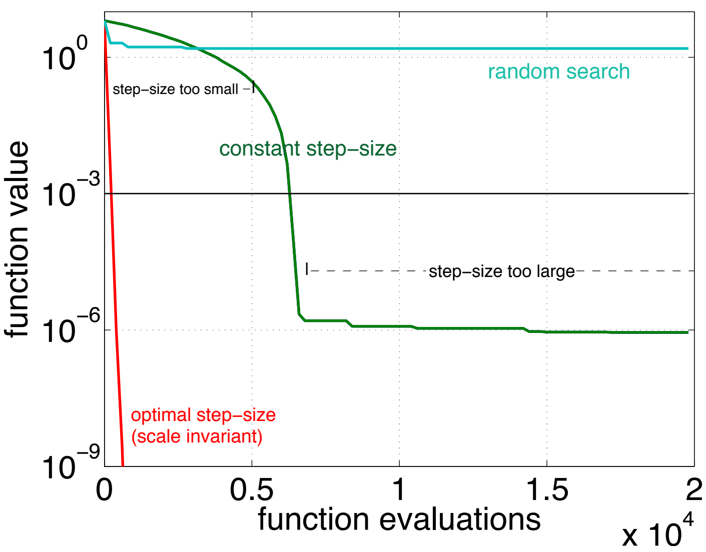
The remaining question is how to update $\mathbf{C}$.

Why Step-Size Control?



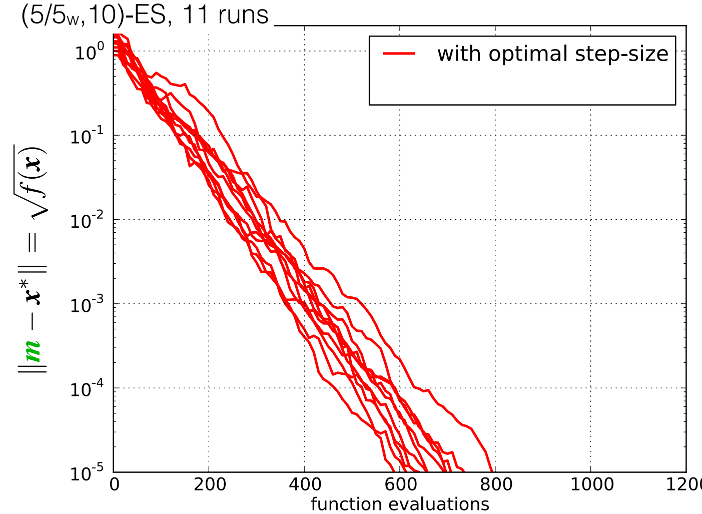
(1+1)-ES
(red & green)

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

in $[-2.2, 0.8]^n$
for $n = 10$

Why Step-Size Control?

(5/5w,10)-ES, 11 runs



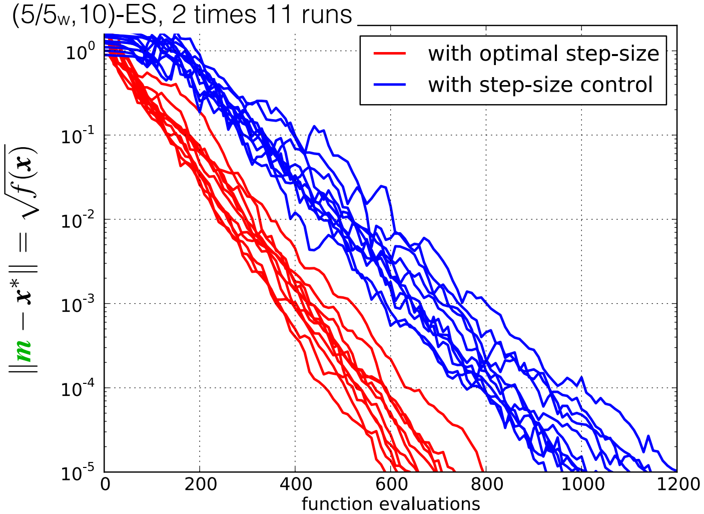
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

for $n = 10$ and
$\boldsymbol{x}^0 \in [-0.2, 0.8]^n$

with optimal step-size σ

Why Step-Size Control?

(5/5w,10)-ES, 2 times 11 runs



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with optimal versus adaptive step-size σ with too small initial σ

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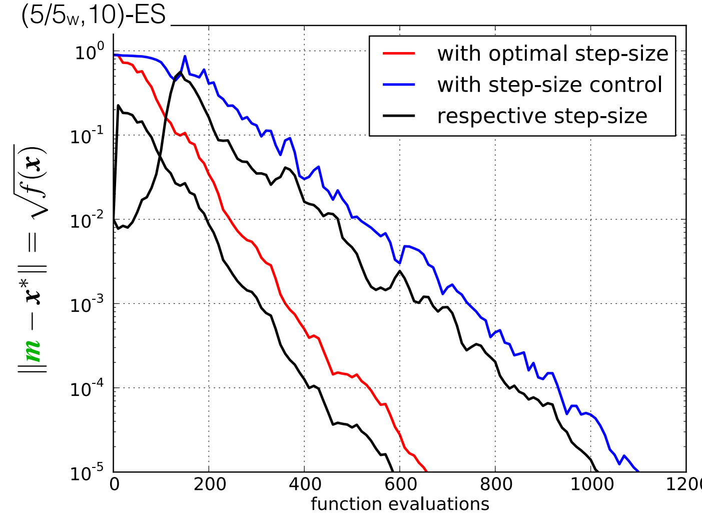
(5/5w,10)-ES



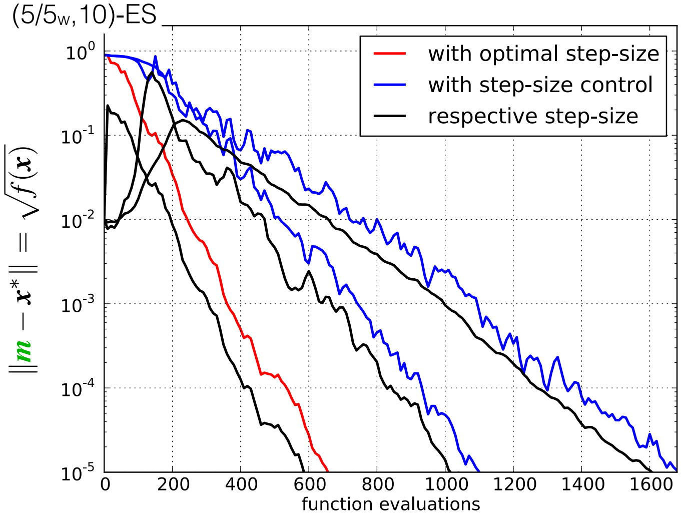
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

for $n = 10$ and
$\boldsymbol{x}^0 \in [-0.2, 0.8]^n$

comparing number of f-evals to reach $\|\boldsymbol{m}\| = 10^{-5}$: $\frac{1100-100}{650} \approx 1.5$

Why Step-Size Control?

(5/5w,10)-ES



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in $[-0.2, 0.8]^n$
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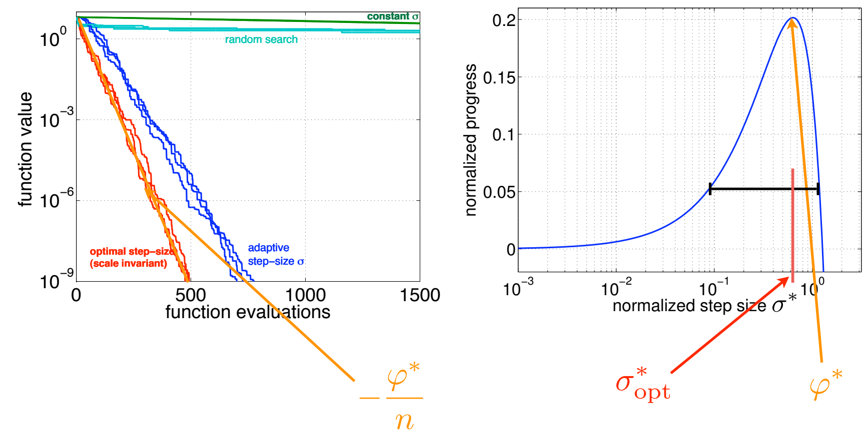
comparing optimal versus default damping parameter d_σ: $\frac{1700}{1100} \approx 1.5$

Why Step-Size Control?

$$\sigma_{\text{opt}} = \sigma^*_{\text{opt}} \frac{\|m\|}{n} \approx \mu_w \frac{\|m\|}{n}$$



evolution window refers to the step-size interval (|——|) where reasonable performance is observed

Methods for Step-Size Control

- $1/5$-th success rule[ab], often applied with "+"-selection

  increase step-size if more than 20% of the new solutions are successful, decrease otherwise
- σ-self-adaptation[c], applied with ","-selection

  mutation is applied to the step-size and the better, according to the objective function value, is selected

  simplified "global" self-adaptation
- path length control[d] (Cumulative Step-size Adaptation, CSA)[e]

  self-adaptation derandomized and non-localized

[a] Rechenberg 1973, *Evolutionsstrategie, Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*, Frommann-Holzboog

[b] Schumer and Steiglitz 1968. Adaptive step size random search. *IEEE TAC*

[c] Schwefel 1981, *Numerical Optimization of Computer Models*, Wiley

[d] Hansen & Ostermeier 2001, Completely Derandomized Self-Adaptation in Evolution Strategies, *Evol. Comput. 9(2)*

[e] Ostermeier *et al* 1994, Step-size adaptation based on non-local use of selection information, *PPSN IV*

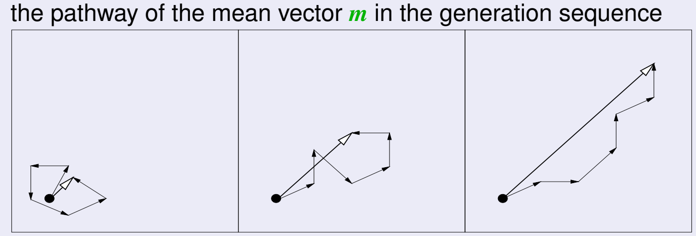
Path Length Control (CSA)

The Concept of Cumulative Step-Size Adaptation

$$\begin{aligned} \boldsymbol{x}_i &= \boldsymbol{m} + \sigma\, \boldsymbol{y}_i \\ \boldsymbol{m} &\leftarrow \boldsymbol{m} + \sigma\, \boldsymbol{y}_w \end{aligned}$$

Measure the length of the *evolution path*

the pathway of the mean vector $\boldsymbol{m}$ in the generation sequence



$\Downarrow$ decrease σ $\qquad$ $\Downarrow$ increase σ

loosely speaking steps are

- perpendicular under random selection (in expectation)
- perpendicular in the desired situation (to be most efficient)

Path Length Control (CSA)

The Equations

Initialize $\boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, evolution path $\boldsymbol{p}_\sigma = \mathbf{0}$,
set $c_\sigma \approx 4/n$, $d_\sigma \approx 1$.

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \quad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda} \qquad \text{update mean}$$

$$\boldsymbol{p}_\sigma \leftarrow (1-c_\sigma)\boldsymbol{p}_\sigma + \underbrace{\sqrt{1-(1-c_\sigma)^2}}_{\text{accounts for } 1-c_\sigma} \underbrace{\sqrt{\mu_w}}_{\text{accounts for } w_i} \boldsymbol{y}_w$$

$$\sigma \leftarrow \sigma \times \underbrace{\exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|}-1\right)\right)}_{>1 \iff \|\boldsymbol{p}_\sigma\| \text{ is greater than its expectation}} \qquad \text{update step-size}$$

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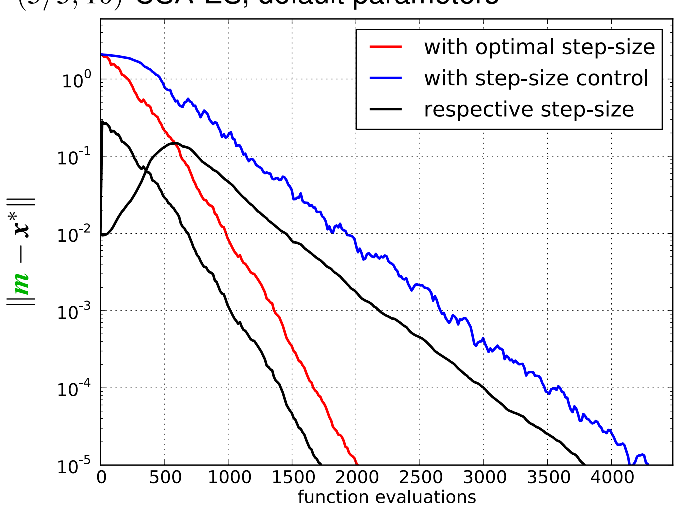
$(5/5, 10)$-CSA-ES, default parameters



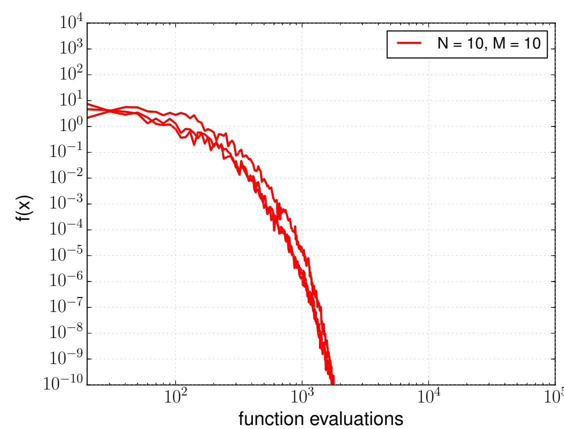
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

in $[-0.2, 0.8]^n$
for $n = 30$

Known Issues of CSA I: With Ineffective Axes

On a function with ineffective axes

- $f(\boldsymbol{x}) = \sum_{i=1}^{M} [\boldsymbol{x}]_i^2$, $\quad \boldsymbol{x} \in \mathbb{R}^N$, $\quad M \le N$.
- $N - M$ variables do not affect the function value



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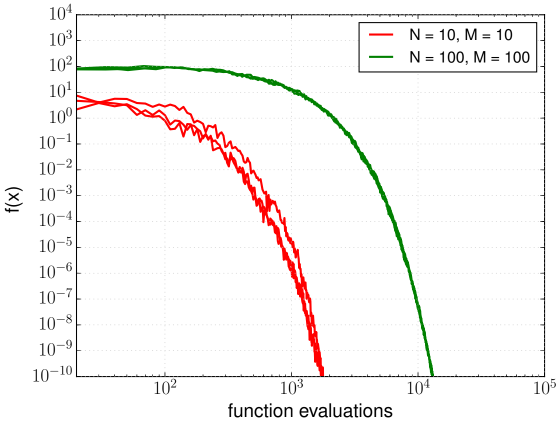

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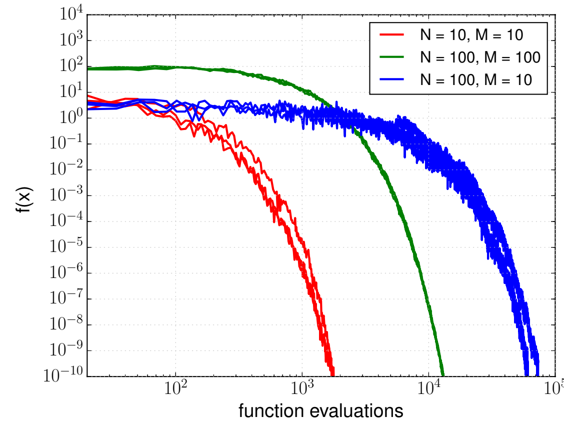

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- $N - M$ variables do not affect the function value

If $M \ll N$,

- The $N - M$ components of $\boldsymbol{p}_\sigma$ are normally distributed
- The signal to change the step size is in the M components

$$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\boldsymbol{p}_\sigma + \sqrt{c_\sigma(2 - c_\sigma)}\sqrt{\mu_w}\sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}$$

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})\|} - 1\right)\right)$$

Known Issues of CSA II: With a Large Population

With large λ and μ

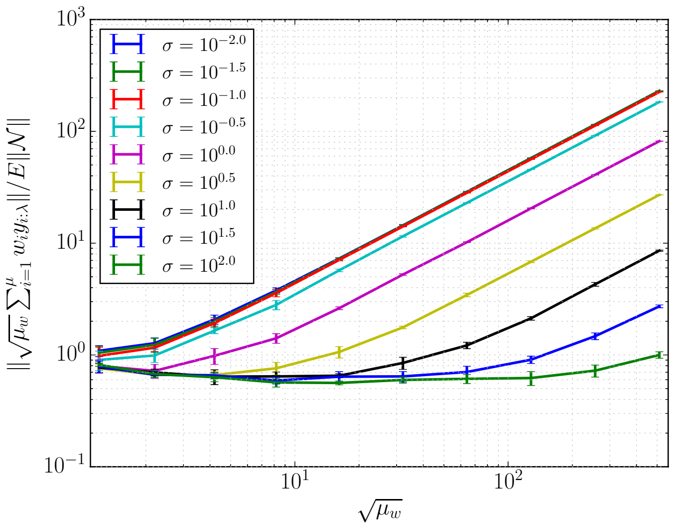
$$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\boldsymbol{p}_\sigma + \sqrt{c_\sigma(2 - c_\sigma)}\underbrace{\sqrt{\mu_w}}_{\propto \mu \to \infty \text{ as } \lambda, \mu \to \infty}\overbrace{\sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}}^{\text{converges to a nonzero constant as } \lambda, \mu \to \infty}$$

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})\|} - 1\right)\right)$$

- $\|\boldsymbol{p}_\sigma\| \propto \sqrt{\mu_w} \quad \Longrightarrow \quad \frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})\|} - 1 \propto \sqrt{\frac{\mu_w}{N}} - 1$ unless $\|\boldsymbol{m} - \boldsymbol{x}^*\| \ll \sigma$
- $d_\sigma \propto \sqrt{\frac{N}{\mu_w}}$ to prevent a increase of σ in one step, however, the convergence will be very slow.

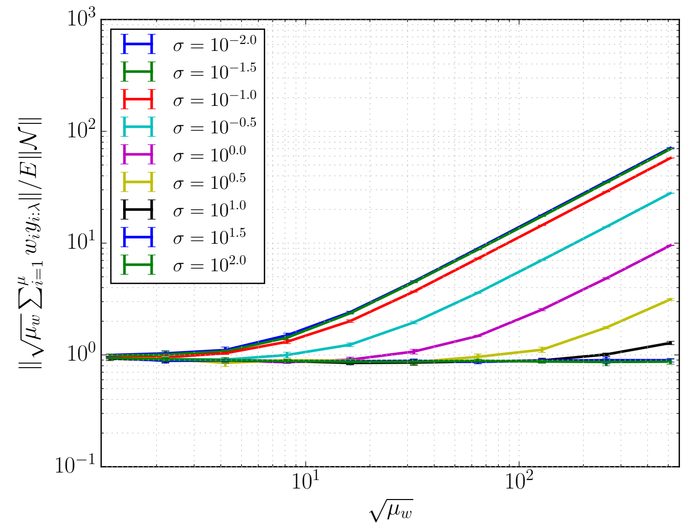
Known Issues of CSA II: With a Large Population

Sphere function ($n = 10$, $\boldsymbol{m} = (1, 0, \dots, 0)$)



Known Issues of CSA II: With a Large Population

Sphere function ($n = 100$, $\boldsymbol{m} = (1, 0, \dots, 0)$)



Two-Point Step-Size Adaptation (TPA)

- Sample a pair of symmetric point along the previous mean shift

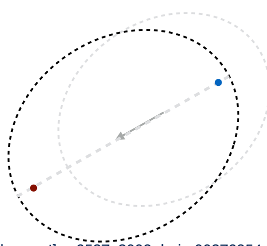
$$\boldsymbol{x}_{1/2} = \boldsymbol{m}^{(g)} \pm \sigma^{(g)} \frac{\|\mathcal{N}(\mathbf{0}, \mathbf{I})\|}{\|\boldsymbol{m}^{(g)} - \boldsymbol{m}^{(g-1)}\|_{\mathbf{C}^{(g)}}} (\boldsymbol{m}^{(g)} - \boldsymbol{m}^{(g-1)}) \qquad \|\boldsymbol{x}\|_{\mathbf{C}} := \boldsymbol{x}^{\mathrm{T}} \mathbf{C}^{-1} \boldsymbol{x}$$

- Compare the ranking of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ among λ current populations

$$s^{(g+1)} = (1 - c_s) s^{(g)} + c_s \underbrace{\frac{\mathrm{rank}(\boldsymbol{x}_2) - \mathrm{rank}(\boldsymbol{x}_1)}{\lambda - 1}}_{>0 \text{ if the previous step still produces a promising solution}}$$

- Update the step-size

$$\sigma^{(g+1)} = \sigma^{(g)} \exp\left(\frac{s^{(g+1)}}{d_\sigma}\right)$$



[Hansen, 2008] Hansen, N. (2008). CMA-ES with two-point step-size adaptation. [research report] rr-6527, 2008. Inria-00276854v5.
[Hansen et al., 2014] Hansen, N., Atamna, A., and Auger, A. (2014). How to assess step-size adaptation mechanisms in randomised search. In Parallel Problem Solving from Nature–PPSN XIII, pages 60–69. Springer.

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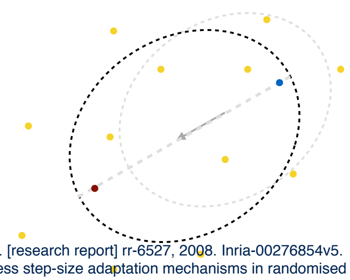

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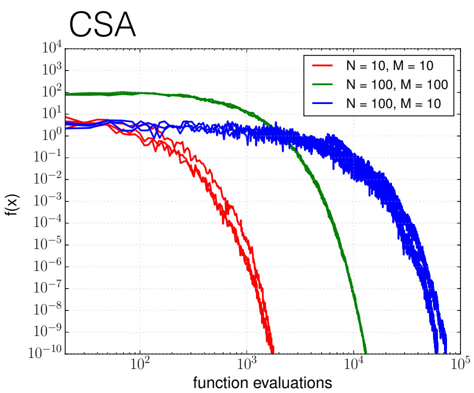

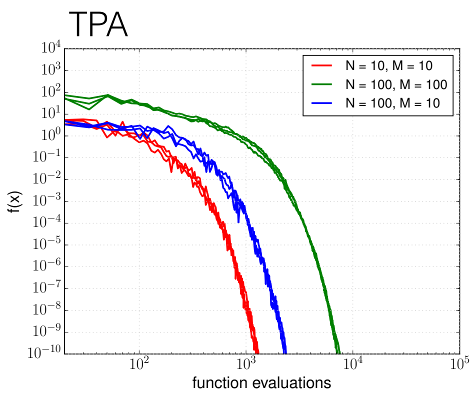

Alternatives: Success-Based Step-Size Control

comparing the fitness distributions of current and previous iterations

Generalizations of $1/5$th-success-rule for non-elitist and multi-recombinant ES

- Median Success Rule [Ait Elhara et al., 2013]
- Population Success Rule [Loshchilov, 2014]

controls a *success probability*

An advantage over CSA and TPA: Cheap Computation

- It depends only on λ.
- cf. CSA and TPA require a computation of $\boldsymbol{C}^{-1/2}\boldsymbol{x}$ and $\boldsymbol{C}^{-1}\boldsymbol{x}$, respectively.

[Ait Elhara et al., 2013] Ait Elhara, O., Auger, A., and Hansen, N. (2013). A median success rule for non- elitist evolution strategies: Study of feasibility. In Proc. of the GECCO, pages 415–422.
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1. Problem Statement
2. Evolution Strategy (ES)
3. Step-Size Adaptation
   - Why Step-Size Control
   - Path Length Control (CSA)
   - Limitations of CSA and its Alternatives
4. Covariance Matrix Adaptation (CMA)
   - Rank-One Update and Cumulation
   - Rank-μ Update
   - Active Covariance Update
5. Design Principle
   - Theoretical Foundations
   - Variants for Large Scale Problems
6. Summary and Final Remarks

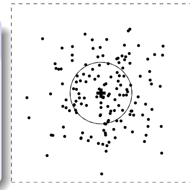
Evolution Strategies

Recalling

New search points are sampled normally distributed

$$x_i \sim m + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \dots, \lambda$$

as perturbations of m, where $x_i, m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



where

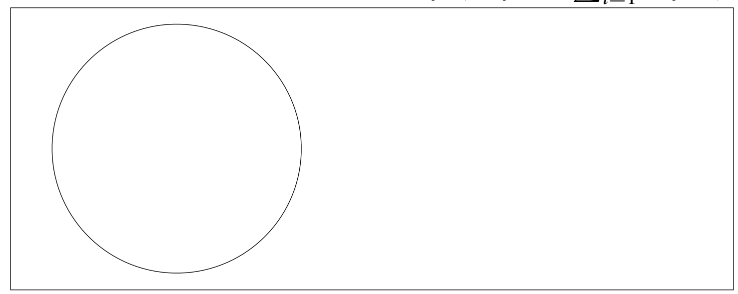
- the mean vector $m \in \mathbb{R}^n$ represents the favorite solution and $m \leftarrow \sum_{i=1}^{\mu} w_i x_{i:\lambda}$
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

The remaining question is how to update σ and $\mathbf{C}$.

Covariance Matrix Adaptation

Rank-One Update

$$m \leftarrow m + \sigma y_w, \quad y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda}, \quad y_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



initial distribution, $\mathbf{C} = \mathbf{I}$

. . . equations

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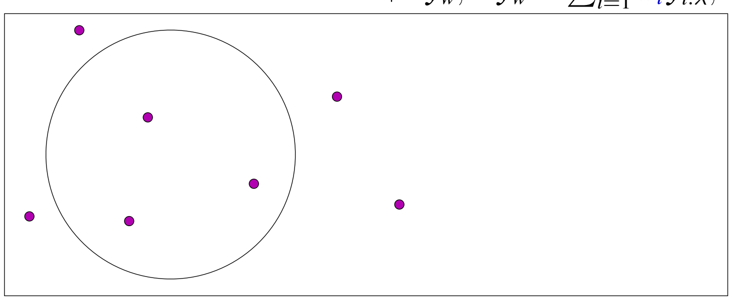

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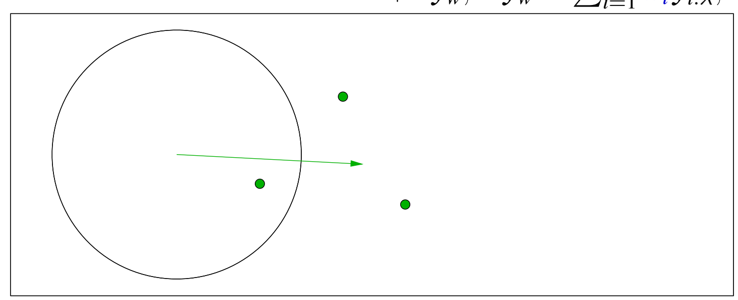

y_w, movement of the population mean m (disregarding σ)

. . . equations

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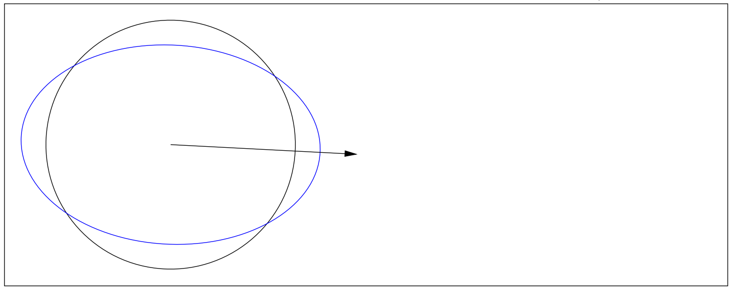

mixture of distribution $\mathbf{C}$ and step y_w,
$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times y_w y_w^{\mathrm{T}}$

...equations

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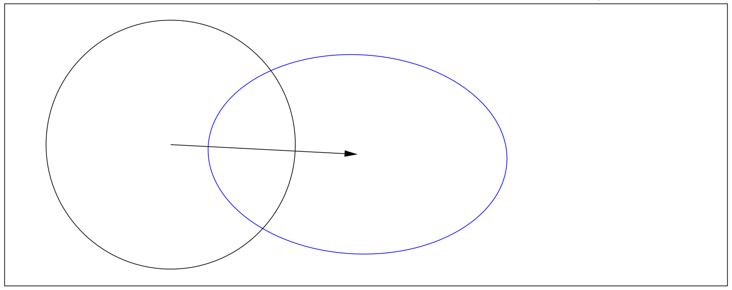

new distribution (disregarding σ)

...equations

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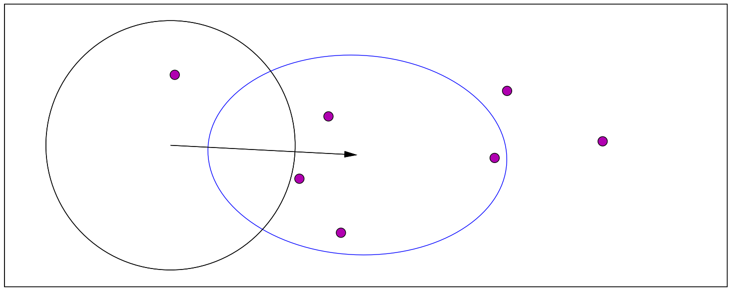

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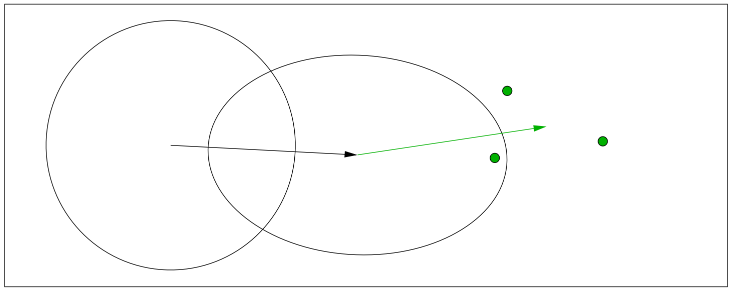

movement of the population mean m

...equations

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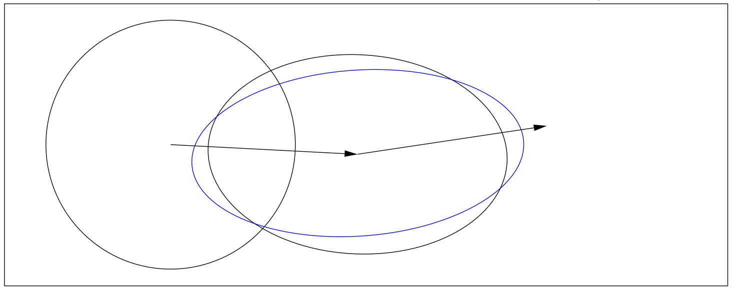

mixture of distribution $\mathbf{C}$ and step $\boldsymbol{y}_w$,

$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

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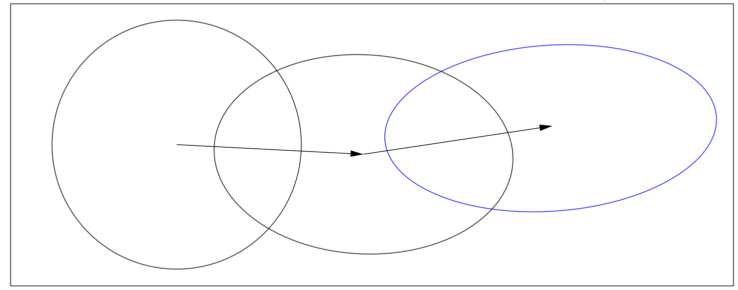


new distribution,

$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

the ruling principle: the adaptation increases the likelihood of successful steps, $\boldsymbol{y}_w$, to appear again

another viewpoint: the adaptation follows a natural gradient approximation of the expected fitness

. . . equations

Covariance Matrix Adaptation

Rank-One Update

Initialize $\boldsymbol{m} \in \mathbb{R}^n$, and $\mathbf{C} = \mathbf{I}$, set $\sigma = 1$, learning rate $c_{\mathrm{cov}} \approx 2/n^2$

While not terminate

$$\boldsymbol{x}_i = \boldsymbol{m} + \sigma \boldsymbol{y}_i, \qquad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}),$$

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \qquad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}$$

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\mathbf{C} + c_{\mathrm{cov}} \mu_w \underbrace{\boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}}_{\text{rank-one}} \qquad \text{where } \mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i^2} \geq 1$$

The rank-one update has been found independently in several domains[6] [7] [8] [9]

[6] Kjellström&Taxén 1981. Stochastic Optimization in System Design, IEEE TCS

[7] Hansen&Ostermeier 1996. Adapting arbitrary normal mutation distributions in evolution strategies: The covariance matrix adaptation, ICEC

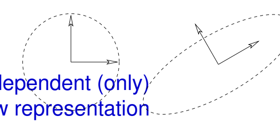
[8] Ljung 1999. System Identification: Theory for the User

[9] Haario et al 2001. An adaptive Metropolis algorithm, JSTOR

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\mathbf{C} + c_{\mathrm{cov}} \mu_w \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$$

covariance matrix adaptation

- learns all pairwise dependencies between variables
  off-diagonal entries in the covariance matrix reflect the dependencies
- conducts a principle component analysis (PCA) of steps $\boldsymbol{y}_w$, sequentially in time and space
  eigenvectors of the covariance matrix $\mathbf{C}$ are the principle components / the principle axes of the mutation ellipsoid
- learns a new rotated problem representation



  components are independent (only) in the new representation
- learns a new (Mahalanobis) metric
  variable metric method
- approximates the inverse Hessian on quadratic functions
  transformation into the sphere function
- for $\mu = 1$: conducts a natural gradient ascent on the distribution $\mathcal{N}$
  entirely independent of the given coordinate system

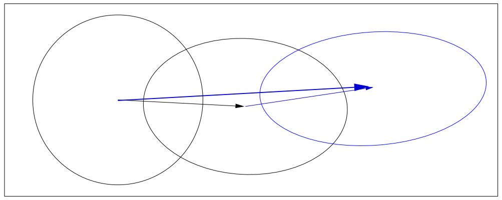
. . . cumulation, rank-μ

Cumulation

The Evolution Path

Evolution Path

Conceptually, the evolution path is the search path the strategy takes over a number of generation steps. It can be expressed as a sum of consecutive *steps* of the mean $\boldsymbol{m}$.



An exponentially weighted sum of steps $\boldsymbol{y}_w$ is used

$$\boldsymbol{p}_c \propto \sum_{i=0}^{g} \underbrace{(1-c_c)^{g-i}}_{\substack{\text{exponentially}\\ \text{fading weights}}} \boldsymbol{y}_w^{(i)}$$

The recursive construction of the evolution path (cumulation):

$$\boldsymbol{p}_c \leftarrow \underbrace{(1-c_c)}_{\text{decay factor}} \boldsymbol{p}_c + \underbrace{\sqrt{1-(1-c_c)^2}\sqrt{\mu_w}}_{\text{normalization factor}} \underbrace{\boldsymbol{y}_w}_{\text{input } = \frac{\boldsymbol{m}-\boldsymbol{m}_{\text{old}}}{\sigma}}$$

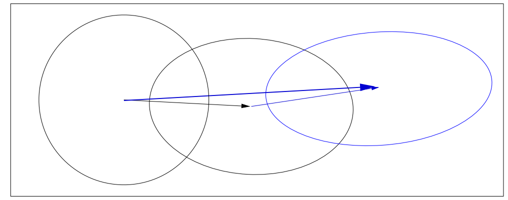
where $\mu_w = \frac{1}{\sum w_i^2}$, $c_c \ll 1$. History information is accumulated in the evolution path.

Cumulation

The Evolution Path

Evolution Path

Conceptually, the evolution path is the search path the strategy takes over a number of generation steps. It can be expressed as a sum of consecutive *steps* of the mean $\boldsymbol{m}$.



An exponentially weighted sum of steps $\boldsymbol{y}_w$ is used

$$\boldsymbol{p}_c \propto \sum_{i=0}^{g} \underbrace{(1-c_c)^{g-i}}_{\substack{\text{exponentially}\\ \text{fading weights}}} \boldsymbol{y}_w^{(i)}$$

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"Cumulation" is a widely used technique and also know as

- *exponential smoothing* in time series, forecasting
- exponentially weighted *mooving average*
- *iterate averaging* in stochastic approximation
- *momentum* in the back-propagation algorithm for ANNs
- ...

"Cumulation" conducts a *low-pass* filtering, but there is more to it...

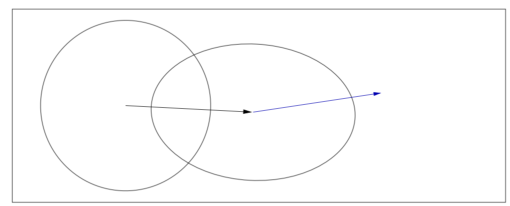
...why?

Cumulation

$$\mathbf{C} \leftarrow (1-c_{\text{cov}})\mathbf{C} + c_{\text{cov}}\mu_w \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$$

Utilizing the Evolution Path

We used $\boldsymbol{y}_w\boldsymbol{y}_w^{\mathrm{T}}$ for updating $\mathbf{C}$. Because $\boldsymbol{y}_w\boldsymbol{y}_w^{\mathrm{T}} = -\boldsymbol{y}_w(-\boldsymbol{y}_w)^{\mathrm{T}}$ the sign of $\boldsymbol{y}_w$ is lost.



The sign information (signifying correlation *between* steps) is (re-)introduced by using the *evolution path*.

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$$\mathbf{C} \leftarrow (1-c_{\text{cov}})\mathbf{C} + c_{\text{cov}} \underbrace{\boldsymbol{p}_c\boldsymbol{p}_c^{\mathrm{T}}}_{\text{rank-one}}$$

where $\mu_w = \frac{1}{\sum w_i^2}$, $c_{\text{cov}} \ll c_c \ll 1$ such that $1/c_c$ is the "backward time horizon".

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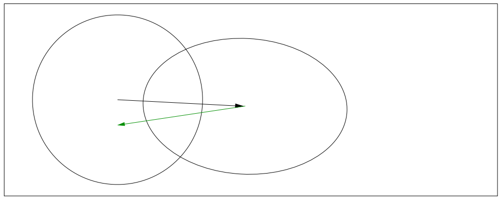

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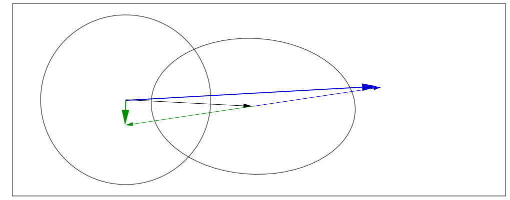

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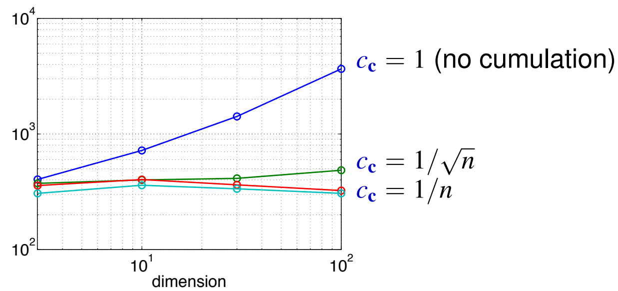
Using an evolution path for the rank-one update of the covariance matrix reduces the number of function evaluations to adapt to a straight ridge from about $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$.[a]

[a] Hansen & Auger 2013. Principled design of continuous stochastic search: From theory to practice.

Number of f-evaluations divided by dimension on the cigar function $f(\boldsymbol{x}) = x_1^2 + 10^6 \sum_{i=2}^n x_i^2$



The overall model complexity is n^2 but important parts of the model can be learned in time of order n

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Rank-μ Update

$$\begin{array}{rclrcl} \boldsymbol{x}_i &=& \boldsymbol{m} + \sigma\,\boldsymbol{y}_i, & \boldsymbol{y}_i &\sim& \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \\ \boldsymbol{m} &\leftarrow& \boldsymbol{m} + \sigma\boldsymbol{y}_w & \boldsymbol{y}_w &=& \sum_{i=1}^{\mu} w_i\,\boldsymbol{y}_{i:\lambda} \end{array}$$

The rank-μ update extends the update rule for large population sizes λ using $\mu > 1$ vectors to update $\mathbf{C}$ at each generation step.
The weighted empirical covariance matrix

$$\mathbf{C}_\mu = \sum_{i=1}^{\mu} w_i\,\boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$$

computes a weighted mean of the outer products of the best μ steps and has rank $\min(\mu, n)$ with probability one.

with $\mu = \lambda$ weights can be negative [10]

The rank-μ update then reads

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\,\mathbf{C} + c_{\mathrm{cov}}\,\mathbf{C}_\mu$$

where $c_{\mathrm{cov}} \approx \mu_w/n^2$ and $c_{\mathrm{cov}} \leq 1$.

[10] Jastrebski and Arnold (2006). Improving evolution strategies through active covariance matrix adaptation. CEC.

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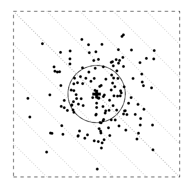
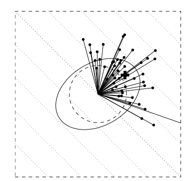


$\boldsymbol{x}_i = \boldsymbol{m} + \sigma\,\boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$

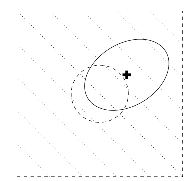
sampling of $\lambda = 150$ solutions where $\mathbf{C} = \mathbf{I}$ and $\sigma = 1$



$\mathbf{C}_\mu = \frac{1}{\mu}\sum \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$

$\mathbf{C} \leftarrow (1 - 1) \times \mathbf{C} + 1 \times \mathbf{C}_\mu$

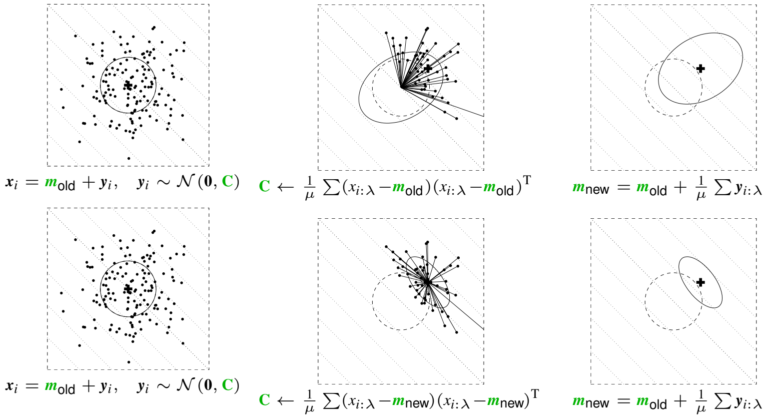
calculating $\mathbf{C}$ where $\mu = 50$, $w_1 = \cdots = w_\mu = \frac{1}{\mu}$, and $c_{\mathrm{cov}} = 1$



$\boldsymbol{m}_{\text{new}} \leftarrow \boldsymbol{m} + \frac{1}{\mu}\sum \boldsymbol{y}_{i:\lambda}$

new distribution

Rank-μ CMA versus Estimation of Multivariate Normal Algorithm EMNA$_{global}$[11]



rank-μ CMA conducts a PCA of steps

EMNA$_{global}$ conducts a PCA of points

sampling of $\lambda = 150$ solutions (dots) | calculating $\mathbf{C}$ from $\mu = 50$ solutions | new distribution

m_{new} is the minimizer for the variances when calculating $\mathbf{C}$

[11] Hansen, N. (2006). The CMA Evolution Strategy: A Comparing Review. In J.A. Lozano, P. Larranga, I. Inza and E. Bengoetxea (Eds.). Towards a new evolutionary computation. Advances in estimation of distribution algorithms. pp. 75-102

The rank-μ update

- increases the possible learning rate in large populations
  roughly from $2/n^2$ to μ_w/n^2
- can reduce the number of necessary generations roughly from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$ (12)
  given $\mu_w \propto \lambda \propto n$

Therefore the rank-μ update is the primary mechanism whenever a large population size is used
say $\lambda \geq 3n + 10$

The rank-one update

- uses the evolution path and reduces the number of necessary function evaluations to learn straight ridges from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$.

Rank-one update and rank-μ update can be combined

...all equations

[12] Hansen, Müller, and Koumoutsakos 2003. Reducing the Time Complexity of the Derandomized Evolution Strategy with Covariance Matrix Adaptation (CMA-ES). *Evolutionary Computation, 11(1)*, pp. 1-18

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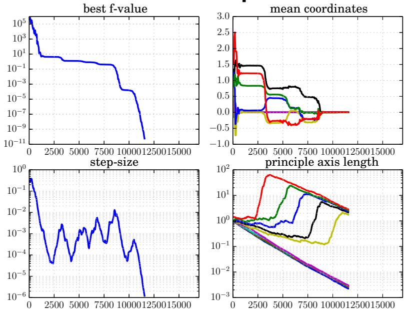
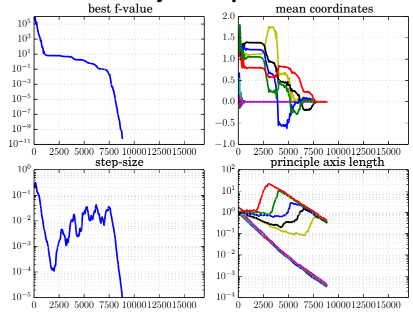
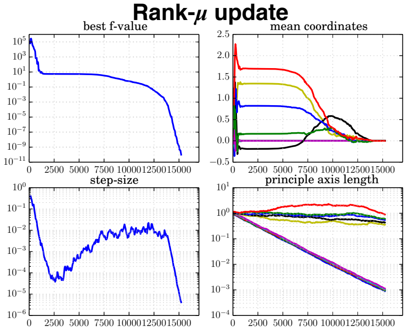


Hybrid update



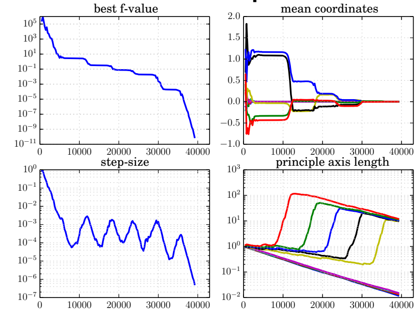
Rank-μ update



$$f_{\text{TwoAxes}}(x) = \sum_{i=1}^{5} x_i^2 + 10^6 \sum_{i=6}^{10} x_i^2$$

$\lambda = 10$ (default for $N = 10$)

Rank-one update



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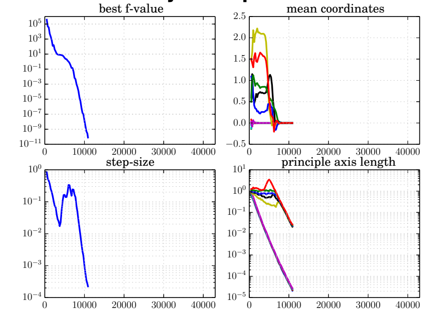
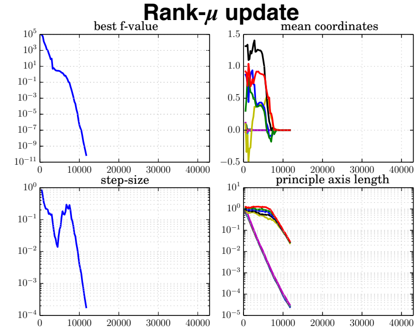


Rank-μ update



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$\lambda = 50$

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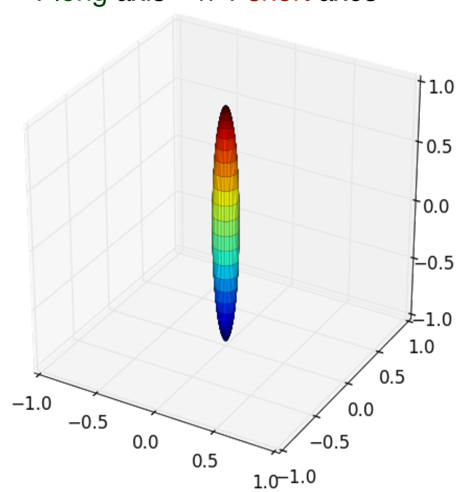
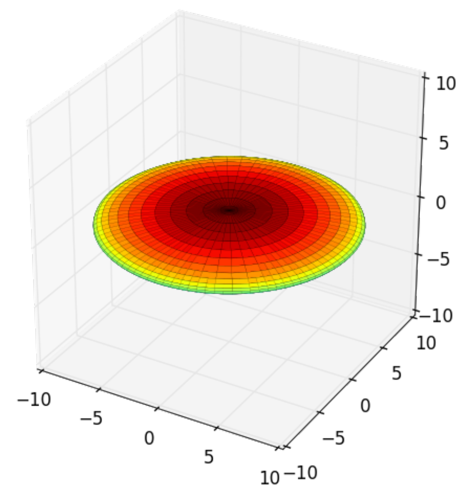
Different Types of Ill-Conditioning

(Axes Ratio = 10)

Cigar Type:
1 long axis = n-1 short axes



Discus Type:
1 short axis = n-1 long axes



Learning a Short/Long Axis

Rank-one and Rank-μ Covariance Matrix Update

$$\boldsymbol{C} \leftarrow (1-c_1-c_\mu)\boldsymbol{C} + \underbrace{c_1 \boldsymbol{p_c}\boldsymbol{p_c}^T + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}}_{\text{nonnegative definite, i.e., increase covariances}}$$

- increases the variance in the directions of $\boldsymbol{p_c}$ and $\boldsymbol{y}_{i:\lambda}$; cumulation is very effective for this purpose
- decrease the variance only by multiplying the factor $(1-c_1-c_\mu)$

Learning a Short/Long Axis

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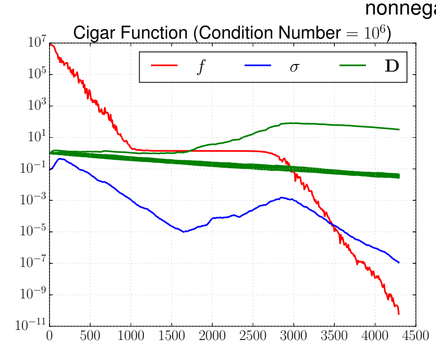
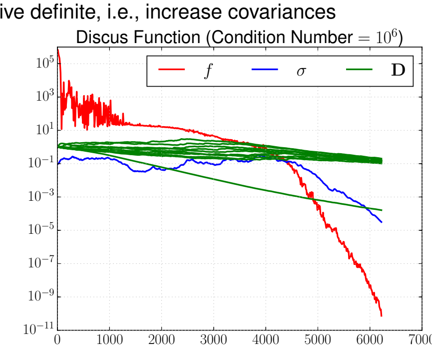




n=10

Active Update

utilize negative weights [Jastrebski and Arnold, 2006]

Rank-one and Rank-μ Active Covariance Matrix Update

$$\boldsymbol{C} \leftarrow (1 - c_1 - c_\mu + c_\mu^-)\boldsymbol{C} + c_1 \boldsymbol{p_c}\boldsymbol{p_c}^T + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}} - c_\mu^- \underbrace{\sum_{i=\lambda-\mu}^{\lambda} |w_i| \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}}_{\text{nonnegative definite}}$$

where

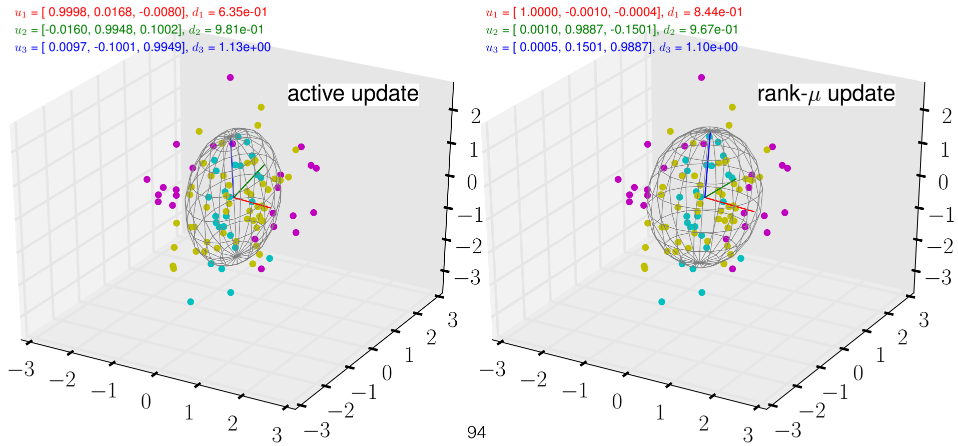
- $-|w_i| < 0$ (for $i \geq \lambda - \mu$): negative weight assigned to $\boldsymbol{y}_{i:\lambda}$, $\sum_{i=\lambda-\mu}^{\lambda} |w_i| = 1$.
- $c_\mu^- > 0$: learning rate for the active update

[Jastrebski and Arnold, 2006] Jastrebski, G. and Arnold, D. V. (2006). Improving Evolution Strategies through Active Covariance Matrix Adaptation. In 2006 IEEE Congress on Evolutionary Computation, pages 9719–9726.

Single Update on Discus Function (n = 3)

$\boldsymbol{C} \leftarrow (1 - c_\mu + c_\mu^-)\boldsymbol{C} + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}} - c_\mu^- \sum_{i=\lambda-\mu}^{\lambda} |w_i| \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$

- $\lambda = 100$, $\mu = \lambda/4$, $w_i = 1/\mu$
- $c_\mu = 0.3$, $c_\mu^- = 0$ for rank-μ update and $c_\mu^- = 0.2$ for active update



Summary

Active Covariance Matrix Adaptation + Cumulation

$$\boldsymbol{C} \leftarrow (1 - c_1 - c_\mu + c_\mu^-)\boldsymbol{C} + c_1 \boldsymbol{p_c}\boldsymbol{p_c}^T + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}} - c_\mu^- \sum_{i=\lambda-\mu}^{\lambda} |w_i| \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$$

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These components compensate each other

- cumulation: excels to learn a long axis, but inefficient for a large λ
- rank-μ update: efficient for a large λ
- active update: effective to learn short axes

An important yet solvable issue of active update

- The positive definiteness of $\boldsymbol{C}$ will be violated if c_μ^- is not small enough
- The positive definiteness can be guaranteed w.p.1 by controlling $c_\mu^- w_i$

Summary

Active Covariance Matrix Adaptation + Cumulation

$$\boldsymbol{C} \leftarrow (1 - c_1 - c_\mu + c_\mu^-)\boldsymbol{C} + c_1 \boldsymbol{p_c}\boldsymbol{p_c}^T + c_\mu \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}} - c_\mu^- \sum_{i=\lambda-\mu}^{\lambda} |w_i| \boldsymbol{y}_{i:\lambda}\boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$$

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- active update: effective to learn short axes

An important yet solvable issue of active update

- The positive definiteness of $\boldsymbol{C}$ will be violated if c_μ^- is not small enough
- The positive definiteness can be guaranteed w.p.1 by controlling $c_\mu^- w_i$

Summary

Active Covariance Matrix Adaptation + Cumulation

$$C \leftarrow (1 - c_1 - c_\mu + c_\mu^-)C + c_1 p_c p_c{}^T + c_\mu \sum_{i=1}^{\mu} w_i y_{i:\lambda} y_{i:\lambda}^T - c_\mu^- \sum_{i=\lambda-\mu}^{\lambda} |w_i| y_{i:\lambda} y_{i:\lambda}^T$$

- $-|w_i| < 0$ (for $i \geq \lambda - \mu$): negative weight assigned to $y_{i:\lambda}$, $\sum_{i=\lambda-\mu}^{\lambda} |w_i| = 1$.
- $c_\mu^- > 0$: learning rate for the active update

These components compensate each other

- cumulation: excels to learn a long axis, but inefficient for a large λ
- rank-μ update: efficient for a large λ
- active update: effective to learn short axes

An important yet solvable issue of active update

- The positive definiteness of C will be violated if c_μ^- is not small enough
- The positive definiteness can be guaranteed w.p.1 by controlling $c_\mu^- w_i$

Summary of Equations

The Covariance Matrix Adaptation Evolution Strategy

Input: $m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, λ (problem dependent)

Initialize: $\mathbf{C} = \mathbf{I}$, and $p_c = \mathbf{0}$, $p_\sigma = \mathbf{0}$,

Set: $c_c \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \leq 1$, $d_\sigma \approx 1 + \sqrt{\frac{\mu_w}{n}}$,
and $w_{i=1\ldots\lambda}$ such that $\mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i^2} \approx 0.3\,\lambda$

While not terminate

$x_i = m + \sigma y_i, \quad y_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \quad$ for $i = 1, \ldots, \lambda$	sampling
$m \leftarrow \sum_{i=1}^{\mu} w_i x_{i:\lambda} = m + \sigma y_w$ where $y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda}$	update mean
$p_c \leftarrow (1 - c_c) p_c + \mathbb{1}_{\{\lVert p_\sigma \rVert < 1.5\sqrt{n}\}} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, y_w$	cumulation for $\mathbf{C}$
$p_\sigma \leftarrow (1 - c_\sigma) p_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} y_w$	cumulation for σ
$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_1 p_c p_c{}^T + c_\mu \sum_{i=1}^{\mu} w_i y_{i:\lambda} y_{i:\lambda}^T$	update $\mathbf{C}$
$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\lVert p_\sigma \rVert}{\mathsf{E}\lVert \mathcal{N}(\mathbf{0},\mathbf{I}) \rVert} - 1\right)\right)$	update of σ

Not covered on this slide: termination, restarts, useful output, boundaries and encoding

Strategy Internal Parameters

- related to selection and recombination
  - λ, offspring number, new solutions sampled, population size
  - μ, parent number, solutions involved in updates of m, $\mathbf{C}$, and σ
  - $w_{i=1,\ldots,\mu}$, recombination weights
- related to $\mathbf{C}$-update
  - c_c, decay rate for the evolution path
  - c_1, learning rate for rank-one update of $\mathbf{C}$
  - c_μ, learning rate for rank-μ update of $\mathbf{C}$
- related to σ-update
  - c_σ, decay rate of the evolution path
  - d_σ, damping for σ-change

Parameters were identified in carefully chosen experimental set ups. Parameters do not in the first place depend on the objective function and are not meant to be in the users choice.
Only(?) the population size λ (and the initial σ) might be reasonably varied in a wide range, *depending on the objective function*
Useful: restarts with increasing population size (IPOP)

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   - Rank-One Update and Cumulation
   - Rank-μ Update
   - Active Covariance Update
5. Design Principle
   - Theoretical Foundations
   - Variants for Large Scale Problems
6. Summary and Final Remarks

Natural Gradient Descend

- Consider $\arg\min_{\boldsymbol{\theta}} \mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$ under the sampling distribution $\boldsymbol{x} \sim p(.|\boldsymbol{\theta})$

  we could improve $\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$ by following the gradient $\nabla_{\boldsymbol{\theta}}\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}}\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta}), \qquad \eta > 0$$

  $\nabla_{\boldsymbol{\theta}}$ depends on the parameterization of the distribution, therefore
- Consider the natural gradient of the expected transformed fitness

$$\begin{aligned}\tilde{\nabla}_{\boldsymbol{\theta}}\mathrm{E}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{\theta}) &= F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}}\mathrm{E}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{\theta}) \\ &= \mathrm{E}(w \circ P_f(f(\boldsymbol{x}))F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}} \ln p(\boldsymbol{x}|\boldsymbol{\theta}))\end{aligned}$$

  using the Fisher information matrix $F_{\boldsymbol{\theta}} = \left(\left(E\frac{\partial^2 \log p(x|\boldsymbol{\theta})}{\partial\theta_i \partial\theta_j}\right)\right)_{ij}$ of the density p.

  The natural gradient is invariant under re-parameterization of the distribution.
- A Monte-Carlo approximation reads

$$\tilde{\nabla}_{\boldsymbol{\theta}}\widehat{\mathrm{E}}(\widehat{w}(f(\boldsymbol{x}))|\boldsymbol{\theta}) = \sum_{i=1}^{\lambda} w_i F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}} \ln p(\boldsymbol{x}_{i:\lambda}|\boldsymbol{\theta}), \quad w_i = \widehat{w}(f(\boldsymbol{x}_{i:\lambda})|\boldsymbol{\theta})$$

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- Consider $\arg\min_{\boldsymbol{\theta}} \mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$ under the sampling distribution $\boldsymbol{x} \sim p(.|\boldsymbol{\theta})$

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Natural Gradient Descend

- Consider $\arg\min_{\theta} \mathrm{E}(f(x)|\theta)$ under the sampling distribution $x \sim p(.|\theta)$ we could improve $\mathrm{E}(f(x)|\theta)$ by following the gradient $\nabla_\theta \mathrm{E}(f(x)|\theta)$:
$$\theta \leftarrow \theta - \eta \nabla_\theta \mathrm{E}(f(x)|\theta), \qquad \eta > 0$$
∇_θ depends on the parameterization of the distribution, therefore
- Consider the natural gradient of the expected transformed fitness
$$\tilde{\nabla}_\theta \mathrm{E}(w \circ P_f(f(x))|\theta) = F_\theta^{-1} \nabla_\theta \mathrm{E}(w \circ P_f(f(x))|\theta)$$
$$= \mathrm{E}(w \circ P_f(f(x)) F_\theta^{-1} \nabla_\theta \ln p(x|\theta))$$
using the Fisher information matrix $F_\theta = \left(\left(E \frac{\partial^2 \log p(x|\theta)}{\partial\theta_i \partial\theta_j}\right)\right)_{ij}$ of the density p.
The natural gradient is invariant under re-parameterization of the distribution.
- A Monte-Carlo approximation reads
$$\tilde{\nabla}_\theta \widehat{\mathrm{E}}(\widehat{w}(f(x))|\theta) = \sum_{i=1}^{\lambda} w_i F_\theta^{-1} \nabla_\theta \ln p(x_{i:\lambda}|\theta), \quad w_i = \widehat{w}(f(x_{i:\lambda})|\theta)$$

CMA-ES = Natural Evolution Strategy + Cumulation

Natural gradient descend using the MC approximation and the normal distribution

- Rewriting the update of the distribution mean
$$m_{\text{new}} \leftarrow \sum_{i=1}^{\mu} w_i x_{i:\lambda} = m + \underbrace{\sum_{i=1}^{\mu} w_i (x_{i:\lambda} - m)}_{\text{natural gradient for mean } \frac{\tilde{\partial}}{\partial m} \widehat{\mathrm{E}}(w \circ P_f(f(x))|m, \mathbf{C})}$$
- Rewriting the update of the covariance matrix[13]
$$\mathbf{C}_{\text{new}} \leftarrow \mathbf{C} + c_1 (\overbrace{p_c p_c^{\mathrm{T}}}^{\text{rank one}} - \mathbf{C})$$
$$+ \underbrace{\frac{c_\mu}{\sigma^2} \sum_{i=1}^{\mu} w_i \left(\overbrace{(x_{i:\lambda} - m)(x_{i:\lambda} - m)^{\mathrm{T}}}^{\text{rank-}\mu} - \sigma^2 \mathbf{C} \right)}_{\text{natural gradient for covariance matrix } \frac{\tilde{\partial}}{\partial \mathbf{C}} \widehat{\mathrm{E}}(w \circ P_f(f(x))|m, \mathbf{C})}$$

[13] Akimoto et.al. (2010): Bidirectional Relation between CMA Evolution Strategies and Natural Evolution Strategies, PPSN XI

Maximum Likelihood Update

The new distribution mean m maximizes the log-likelihood
$$m_{\text{new}} = \arg\max_{m} \sum_{i=1}^{\mu} w_i \log p_{\mathcal{N}}(x_{i:\lambda}|m)$$
independently of the given covariance matrix

$\log p_{\mathcal{N}}(x|m, \mathbf{C}) = -\frac{1}{2} \log \det(2\pi \mathbf{C}) - \frac{1}{2} (x - m)^{\mathrm{T}} \mathbf{C}^{-1} (x - m)$
$p_{\mathcal{N}}$ is the density of the multi-variate normal distribution

Maximum Likelihood Update

The new distribution mean m maximizes the log-likelihood
$$m_{\text{new}} = \arg\max_{m} \sum_{i=1}^{\mu} w_i \log p_{\mathcal{N}}(x_{i:\lambda}|m)$$
independently of the given covariance matrix

The rank-μ update matrix $\mathbf{C}_\mu$ maximizes the log-likelihood
$$\mathbf{C}_\mu = \arg\max_{\mathbf{C}} \sum_{i=1}^{\mu} w_i \log p_{\mathcal{N}} \left(\frac{x_{i:\lambda} - m_{\text{old}}}{\sigma} \middle| m_{\text{old}}, \mathbf{C} \right)$$

$\log p_{\mathcal{N}}(x|m, \mathbf{C}) = -\frac{1}{2} \log \det(2\pi \mathbf{C}) - \frac{1}{2} (x - m)^{\mathrm{T}} \mathbf{C}^{-1} (x - m)$
$p_{\mathcal{N}}$ is the density of the multi-variate normal distribution

CMA-ES as a Natural Gradient

$\mathcal{O}(\lambda N^2)$ floating point (FP) multiplication + $\mathcal{O}(N^2 + \lambda N)$ FP memory. ($\lambda \in o(N)$)

1. $\sqrt{C^{(t)}} = \text{MATRIXSQRT}(C^{(t)})$ (perform every $\mathcal{O}(N/\lambda)$ iter.)
2. $z_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ for $i = 1, \dots, \lambda$
3. $x_i = m^{(t)} + \sigma^{(t)} \sqrt{C^{(t)}} z_i$

$\mathcal{O}(\lambda N^2)$

4. $(x_{i:\lambda})_{i=1,\dots,\lambda} = \text{SORTW.R.T.}^f((x_i)_{i=1,\dots,\lambda})$

5. $p_c^{(t+1)} = (1 - c_c) p_c^{(t)} + \sqrt{c_c(2 - c_c)/(\sum w_i^2)} \sum_{i=1}^{\lambda} w_i (x_{i:\lambda} - m^{(t)})/\sigma^{(t)}$
6. $p_\sigma^{(t+1)} = (1 - c_\sigma) p_\sigma^{(t)} + \sqrt{c_\sigma(2 - c_\sigma)/(\sum w_i^2)} \sum_{i=1}^{\lambda} w_i z_{i:\lambda}$
7. $\sigma^{(t+1)} = \sigma^{(t)} \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|p_\sigma^{(t+1)}\|}{\mathrm{E}\|\mathcal{N}(\mathbf{0}, \boldsymbol{I})\|} - 1\right)\right)$

$\mathcal{O}(\lambda N)$

8. $m^{(t+1)} = m^{(t)} + \sum_{i=1}^{\lambda} w_i \tilde{\nabla} J(x_{i:\lambda})$
9. $C^{(t+1)} = C^{(t)} + c_\mu \sum_{i=1}^{\lambda} w_i \tilde{\nabla} J(x_{i:\lambda}) + c_1 \tilde{\nabla} J(m^{(t)} + \sigma^{(t)} p_c^{(t+1)})$

$\mathcal{O}(\lambda N^2)$

Bottleneck of the CMA-ES

1. $\mathcal{O}(N^2)$ Time and Space Complexities
   - to store and update $C \in \mathbb{R}^{N \times N}$
   - to compute the eigen decomposition of C
2. $\mathcal{O}(1/N^2)$ Learning Rates for C-Update
   - $c_\mu \approx \mu_w / N^2$
   - $c_1 \approx 2/N^2$

$\Rightarrow$ Design a variant of CMA-ES for high dimensional search space

Variants with Restricted Covariance Matrix

CMA-ES Variants with Restricted Covariance Matrices

- Sep-CMA [Ros and Hansen, 2008]
  - $C = \mathbf{D}$. $\mathbf{D}$: Diagonal
- VD-CMA [Akimoto et al., 2014]
  - $C = \mathbf{D}(\mathbf{I} + vv^{\mathrm{T}})\mathbf{D}$. $\mathbf{D}$: Diagonal, $v \in \mathbb{R}^N$.
- LM-CMA [Loshchilov, 2014]
  - $C = \mathbf{I} + \sum_{i=1}^{k} v_i v_i^{\mathrm{T}}$. $v_i \in \mathbb{R}^N$.
- VkD-CMA [Akimoto and Hansen, 2016]
  - $C = \mathbf{D}(\mathbf{I} + \sum_{i=1}^{k} v_i v_i^{\mathrm{T}})\mathbf{D}$. $v_i \in \mathbb{R}^N$.

[Ros and Hansen, 2008] Ros, R. and Hansen, N. (2008). A simple modification in CMA-ES achieving linear time and space complexity. In Parallel Problem Solving from Nature - PPSN X, pages 296–305. Springer.
[Akimoto et al., 2014] Akimoto, Y., Auger, A., and Hansen, N. (2014). Comparison-based natural gradient optimization in high dimension. In Proceedings of Genetic and Evolutionary Computation Conference, pages 373–380, Vancouver, BC, Canada.
[Loshchilov, 2014] Loshchilov, I. (2014). A computationally efficient limited memory cma-es for large scale optimization. In Proceedings of Genetic and Evolutionary Computation Conference, pages 397–404.
[Akimoto and Hansen, 2016] Akimoto, Y. and Hansen, N. (2016). Projection-based restricted covariance matrix adaptation for high dimension. In Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, Colorado, USA, July 20-24, 2016, page (accepted). ACM.

CMA-ES as a Natural Gradient

1. $\sqrt{C^{(t)}} = \text{MATRIXSQRT}(C^{(t)})$ (perform every $\mathcal{O}(N/\lambda)$ iter.)
2. $z_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ for $i = 1, \dots, \lambda$
3. $x_i = m^{(t)} + \sigma^{(t)} \sqrt{C^{(t)}} z_i$

4. $(x_{i:\lambda})_{i=1,\dots,\lambda} = \text{SORTW.R.T.}^f((x_i)_{i=1,\dots,\lambda})$

5. $p_c^{(t+1)} = (1 - c_c) p_c^{(t)} + \sqrt{c_c(2 - c_c)/(\sum w_i^2)} \sum_{i=1}^{\lambda} w_i (x_{i:\lambda} - m^{(t)})/\sigma^{(t)}$
6. $p_\sigma^{(t+1)} = (1 - c_\sigma) p_\sigma^{(t)} + \sqrt{c_\sigma(2 - c_\sigma)/(\sum w_i^2)} \sum_{i=1}^{\lambda} w_i z_{i:\lambda}$
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$\mathcal{O}(\lambda N^2)$ floating point (FP) multiplication + $\mathcal{O}(N^2 + \lambda N)$ FP memory. ($\lambda \in o(N)$)

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$\mathcal{O}(\lambda N^2)$

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$\mathcal{O}(\lambda N)$

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$\mathcal{O}(\lambda N^2)$

Sep-CMA-ES as a Natural Gradient

$\mathcal{O}(\lambda N)$ floating point (FP) multiplication + $\mathcal{O}(N + \lambda N)$ FP memory. ($\lambda \in o(N)$)

1. $\sqrt{C^{(t)}} = \text{MatrixSqrt}(C^{(t)})$
2. $z_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ for $i = 1, \dots, \lambda$
3. $x_i = m^{(t)} + \sigma^{(t)} \sqrt{C^{(t)}} z_i$

$\mathcal{O}(\lambda N)$

4. $(x_{i:\lambda})_{i=1,\dots,\lambda} = \text{SortW.R.T.}^f((x_i)_{i=1,\dots,\lambda})$
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$\mathcal{O}(\lambda N)$

Plug diagonal C and compute the natural gradient

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The Continuous Search Problem

Difficulties of a non-linear optimization problem are

- dimensionality and non-separabitity
  demands to exploit problem structure, e.g. neighborhood
  cave: design of benchmark functions
- ill-conditioning
  demands to acquire a second order model
- ruggedness
  demands a non-local (stochastic? population based?) approach

Main Characteristics of (CMA) Evolution Strategies

1. Multivariate normal distribution to generate new search points
   follows the maximum entropy principle
2. Rank-based selection
   implies invariance, same performance on $g(f(\boldsymbol{x}))$ for any increasing g
   more invariance properties are featured
3. Step-size control facilitates fast (log-linear) convergence and possibly linear scaling with the dimension
   in CMA-ES based on an evolution path (a non-local trajectory)
4. *Covariance matrix adaptation (CMA)* increases the likelihood of previously successful steps and can improve performance by orders of magnitude
   the update follows the natural gradient
   $\mathbf{C} \propto \boldsymbol{H}^{-1} \iff$ adapts a variable metric
   $\iff$ new (rotated) problem representation
   $\Longrightarrow f : \boldsymbol{x} \mapsto g(\boldsymbol{x}^{\mathrm{T}}\boldsymbol{H}\boldsymbol{x})$ reduces to $\boldsymbol{x} \mapsto \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}$

Limitations

of CMA Evolution Strategies

- internal CPU-time: $10^{-8}n^2$ seconds per function evaluation on a 2GHz PC, tweaks are available
  1 000 000 f-evaluations in 100-D take 100 seconds *internal* CPU-time
- better methods are presumably available in case of
  - partly separable problems
  - specific problems, for example with cheap gradients
    specific methods
  - small dimension ($n \ll 10$)
    for example Nelder-Mead
  - small running times (number of f-evaluations $< 100n$)
    model-based methods

Thank You

Source code for CMA-ES in C, Java, Matlab, Octave, Python, Scilab is available at `http://www.lri.fr/~hansen/cmaes_inmatlab.html`